

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 327 °C

Global applicability domain: Inside

Local applicability domain index: 5.78e-01

Confidence level: 7.85e-01

Nearest Neighbors from the Training Set

Image not found

2,4-Dimethylbenzophenone

Measured: 322

Predicted: 327

Image not found

3,4-Dimethylbenzophenone

Measured: 341

Predicted: 327

Image not found

Methanone, bis(4-methylphenyl)-

Measured: 334

Predicted: 327

Image not found

2-Propanone, 1,1-diphenyl-

Measured: 307

Predicted: 327